

Procedure for Modeling Complexes

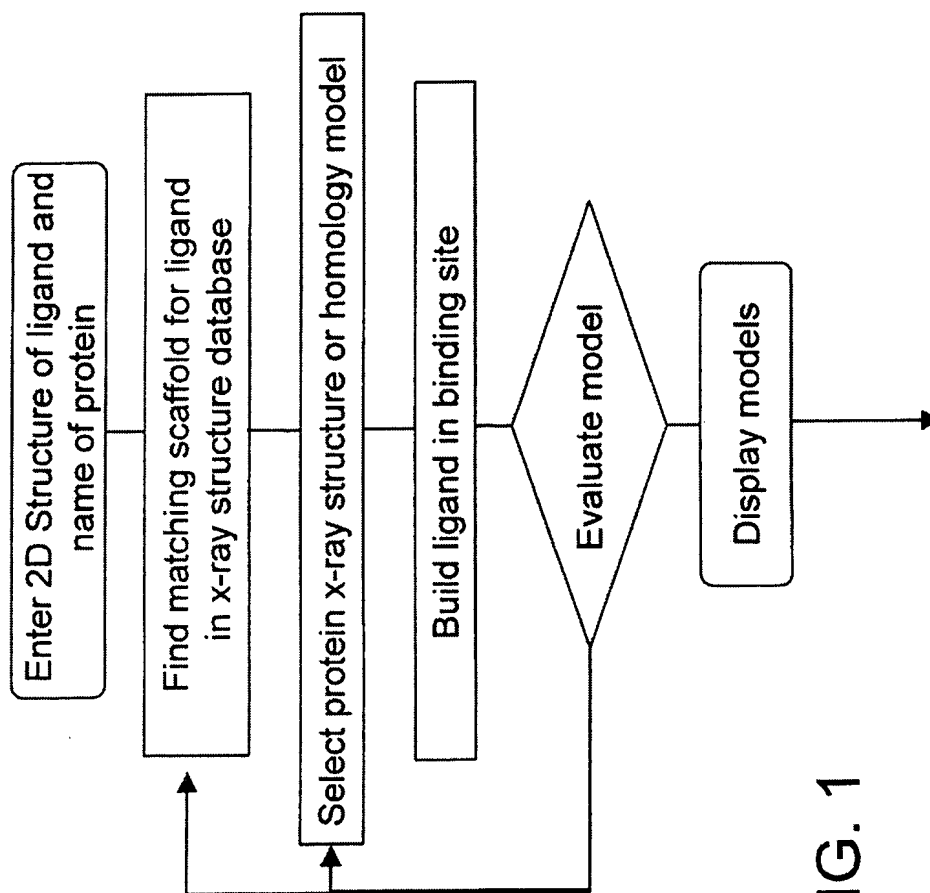
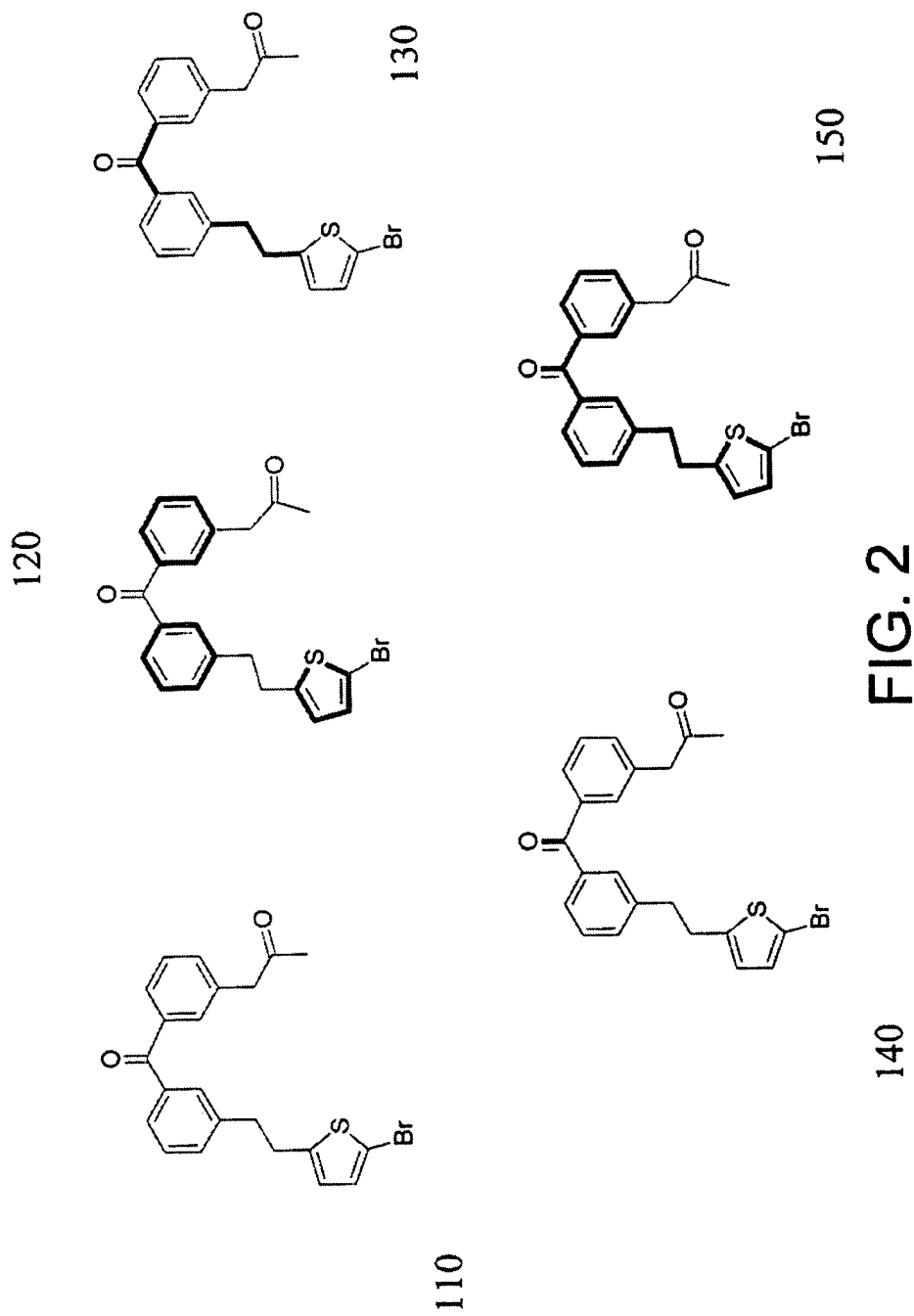


FIG. 1



Maximum Common Substructure

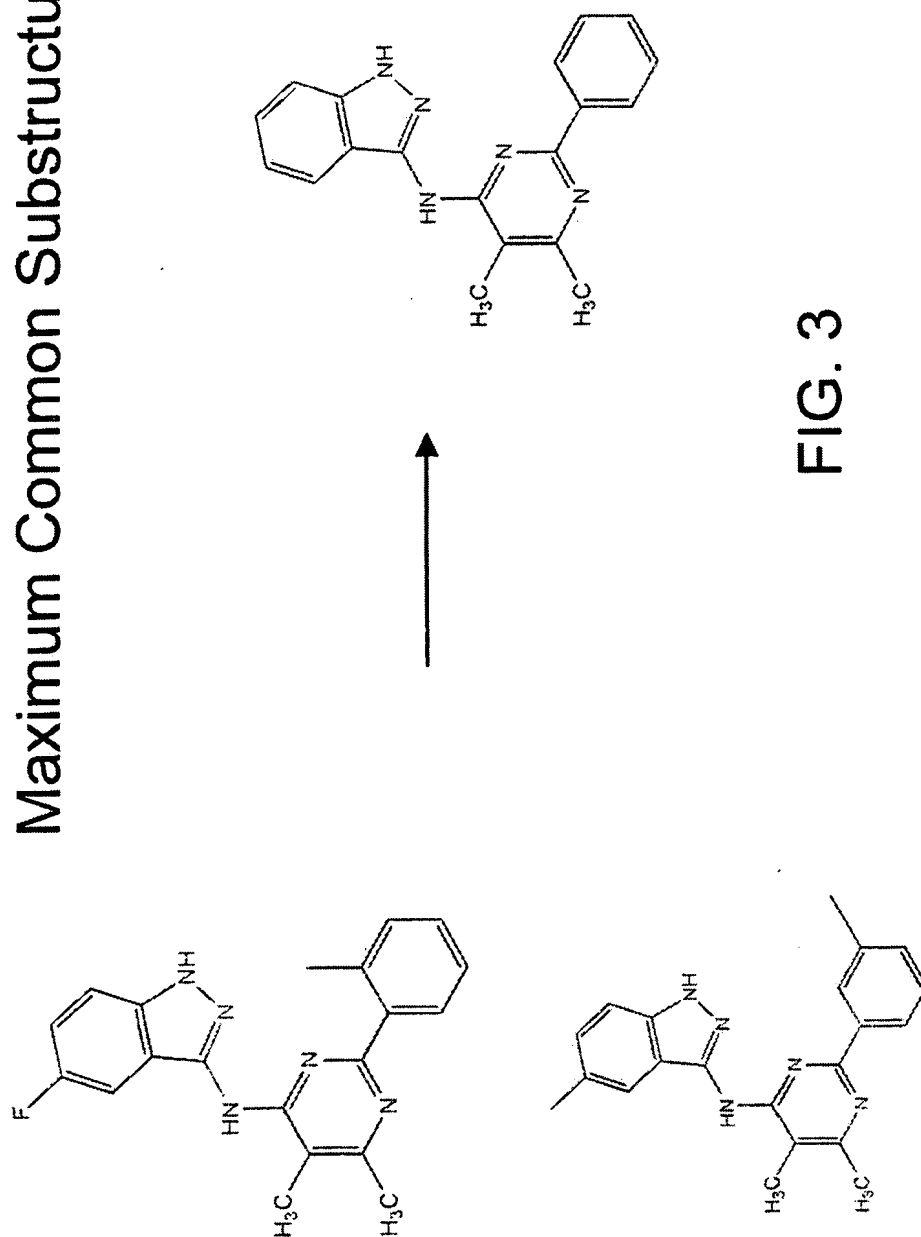


FIG. 3

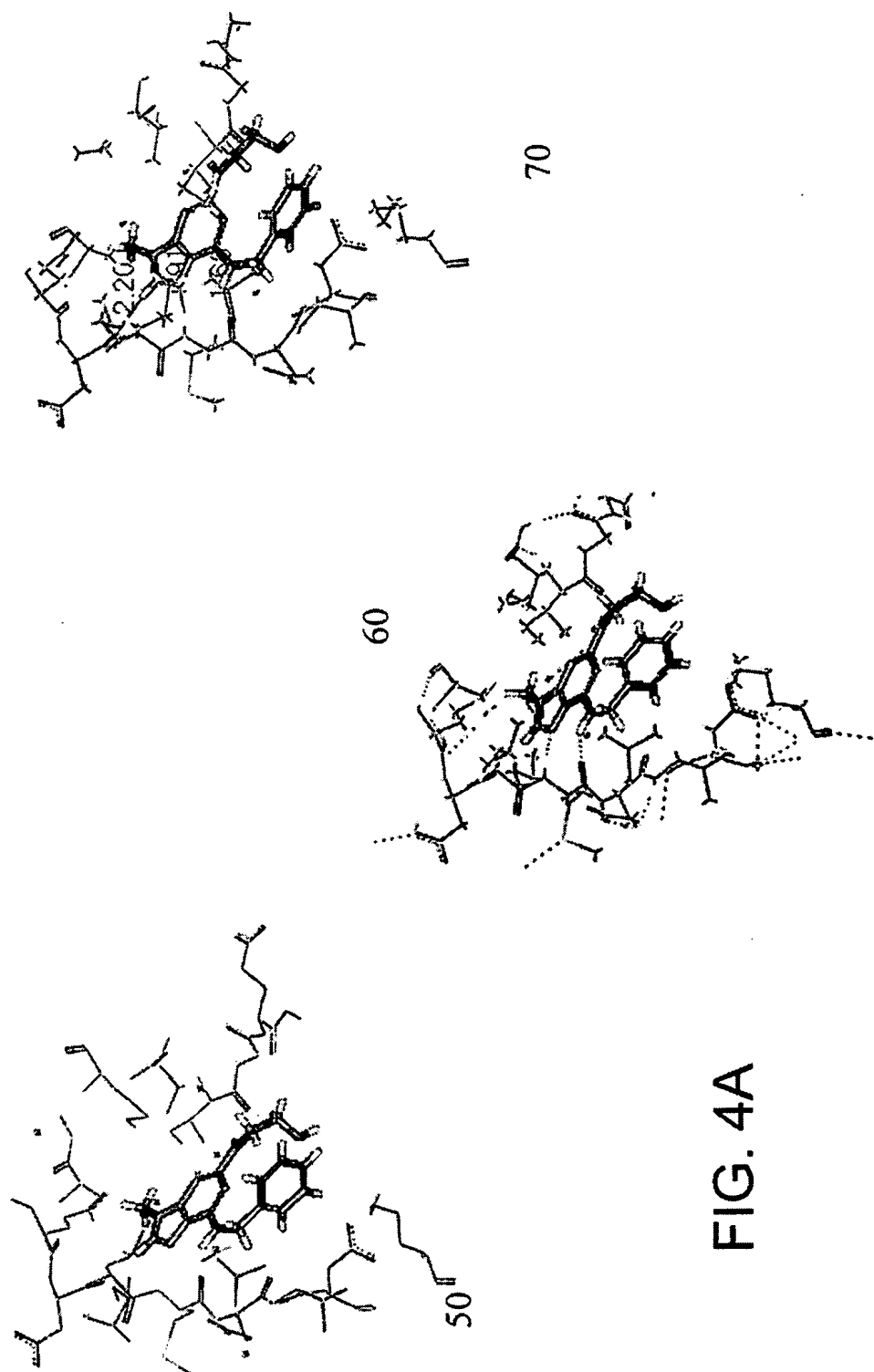
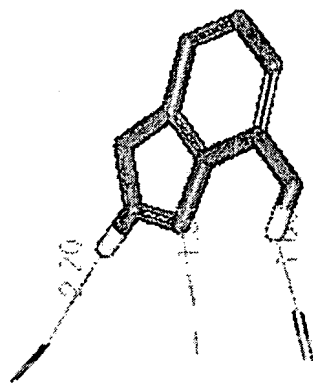
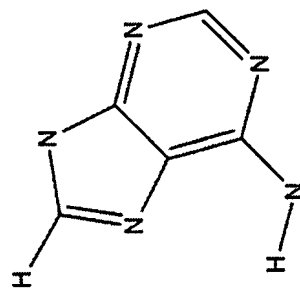


FIG. 4A

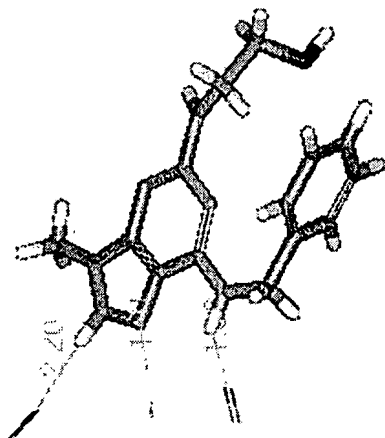


90

FIG. 4B



100



80

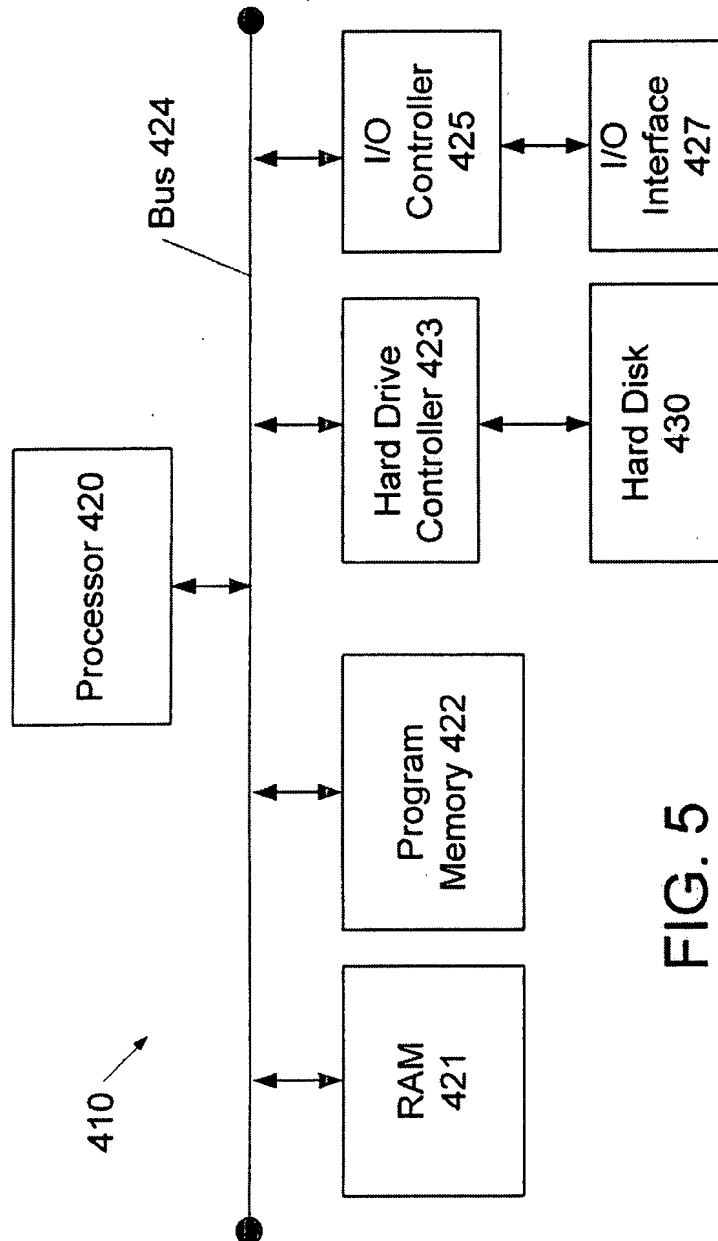


FIG. 5

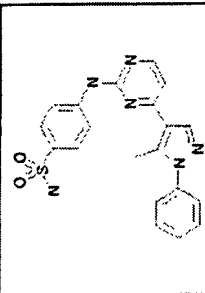
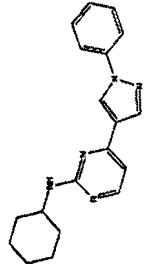
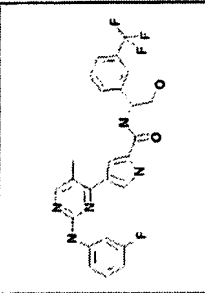
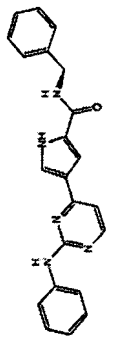
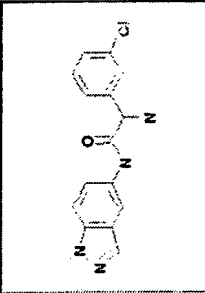
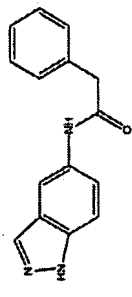
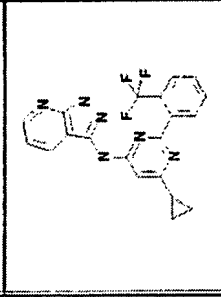
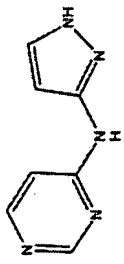
| query ligand | protein | scaffold | rmsd (model vs. x-ray) / Angstrom |
|---|----------|--|--------------------------------------|
|  | jnk3 |  | 0.9 – 1.3 |
|  | erk2 |  | 1.5 – 2.0 |
|  | pka(5xm) |  | 1.2 |
|  | gsk3β |  | 1.3 – 2.2 |

FIG. 6

FIG. 7A

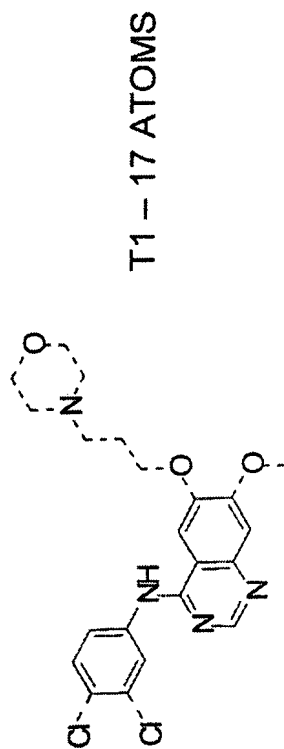


FIG. 7B

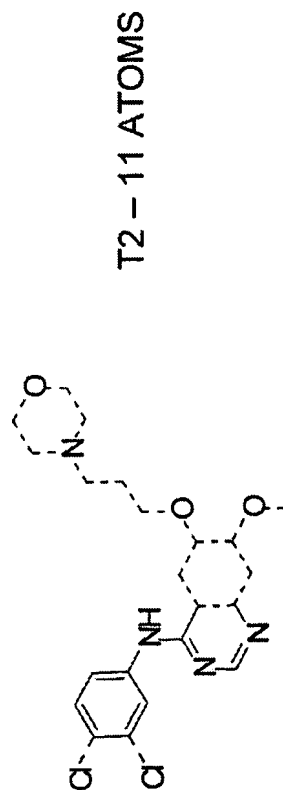
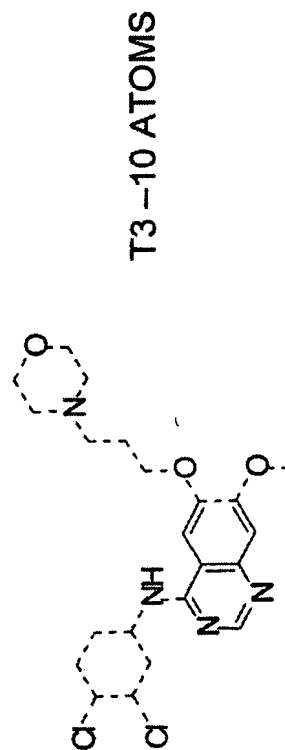


FIG. 7C



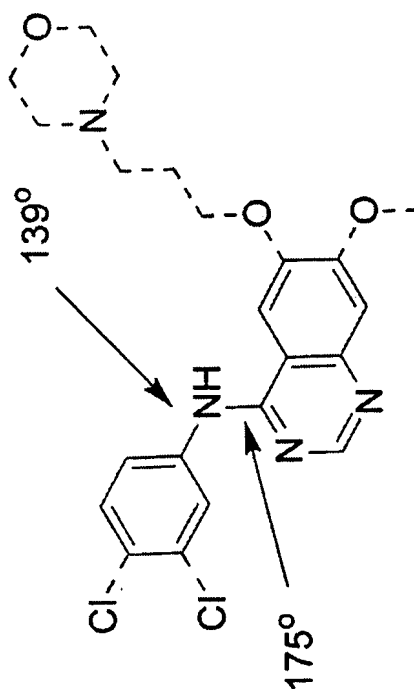


FIG. 8

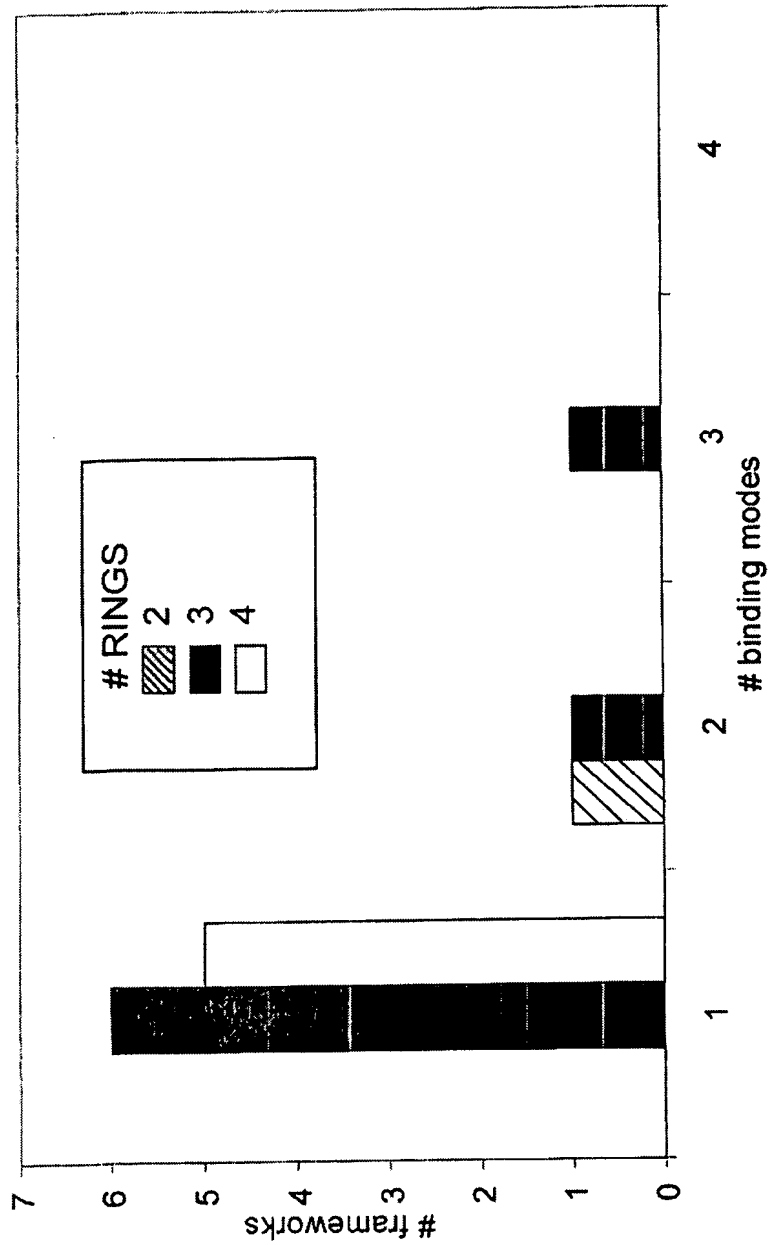


FIG. 9

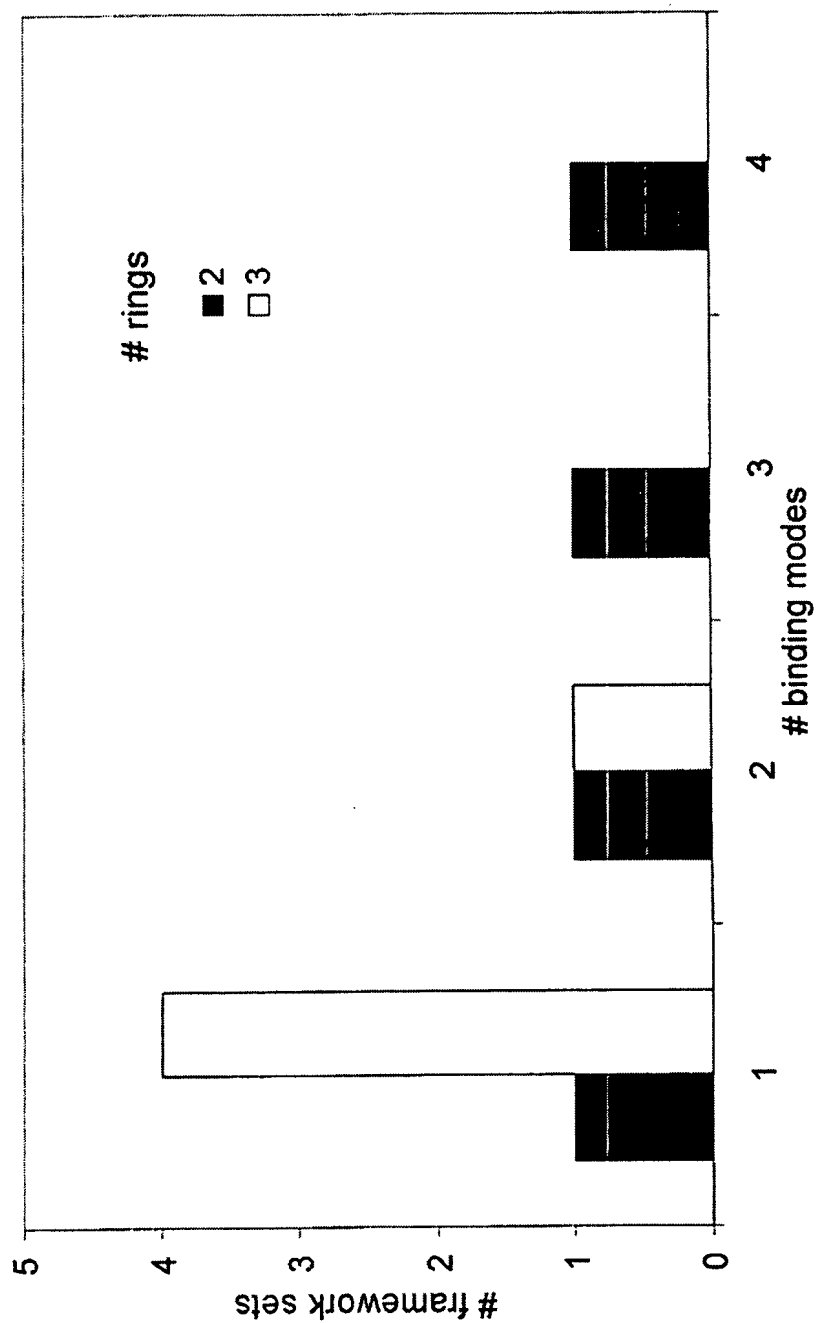


FIG. 10

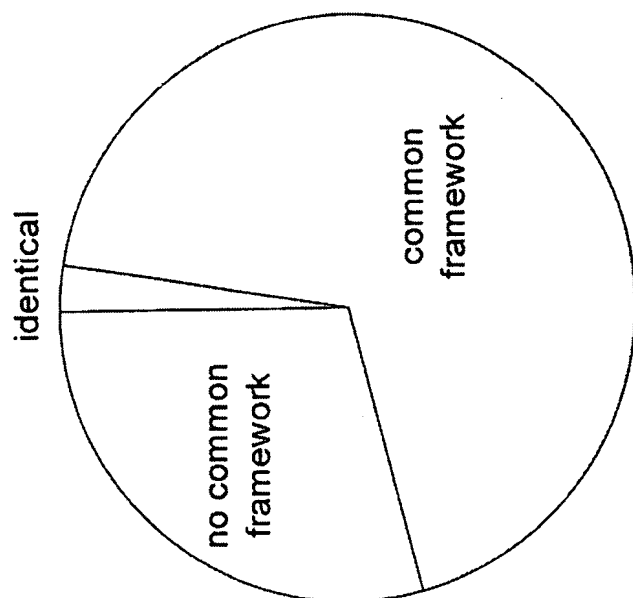


FIG. 11

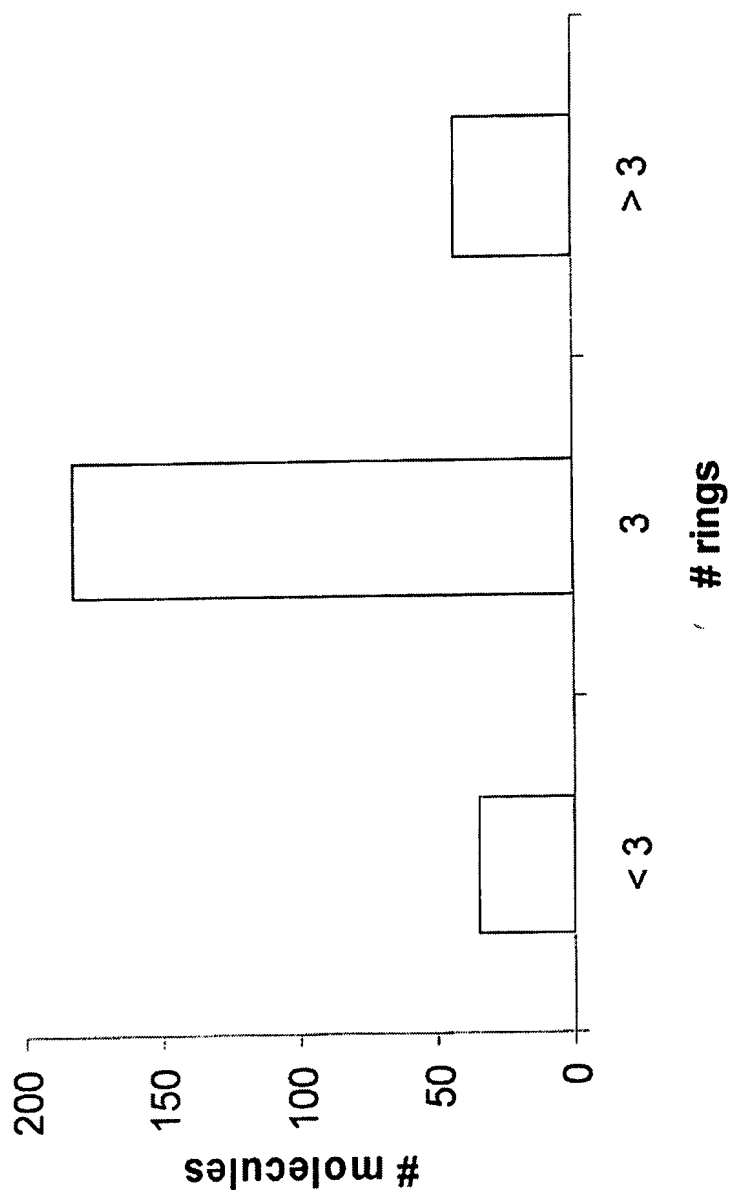
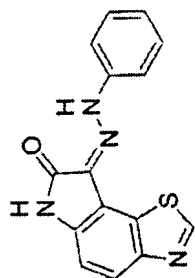
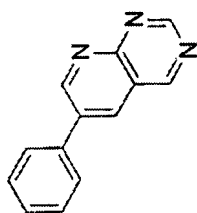


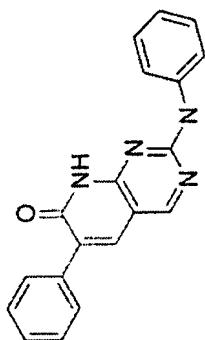
FIG. 12



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FIG. 13